MPI Optimisation

Advanced Message-Passing Programming

Engineering and Physical Sciences Research Council
Natural Environment Research Council

Reusing this material

Overview

Can divide overheads up into four main categories:

- Lack of parallelism
- Load imbalance
- Synchronisation
- Communication

Lack of parallelism

- Tasks may be idle because only a subset of tasks are computing
- Could be one task only working, or several.
  - work done on task 0 only
  - with split communicators, work done only on task 0 of each communicator
- Usually, the only cure is to redesign the algorithm to exploit more parallelism.

Load imbalance

- All tasks have some work to do, but some more than others....
- In general a much harder problem to solve than in shared variables model
  - need to move data explicitly to where tasks will execute
- May require significant algorithmic changes to get right
- Again scaling to large processor counts may be hard
  - the load balancing algorithms may themselves scale as O(p) or worse.

- MPI profiling tools report the amount of time spent in each MPI routine
- For blocking routines (e.g. Recv, Wait, collectives) this time may be a result of load imbalance.
- The task is blocked waiting for another task to enter the corresponding MPI call
  - the other tasks may be late because it has more work to do
- Tracing tools often show up load imbalance very clearly
  - but may be impractical for large codes, large task counts, long runtimes

Synchronisation

- In MPI most synchronisation is coupled to communication
  - Blocking sends/receives
  - Waits for non-blocking sends/receives
  - Collective comms are (mostly) synchronising
- MPI_Barrier is almost never required for correctness
  - can be useful for timing
  - can be useful to prevent buffer overflows if one task is sending a lot of messages and the receiving task(s) cannot keep up.
  - think carefully why you are using it!
- Use of blocking point-to-point comms can result in unnecessary synchronisation.
  - Can amplify “random noise” effects (e.g. OS interrupts)

Communication

- Point-to-point communications
- Collective communications

Small messages

- Point to point communications typically incur a start-up cost
  - sending a 0 byte message takes a finite time
- Time taken for a message to transit can often be well modeled as

$$T_p = T_l + N_b T_b$$

where T_l is start-up cost or *latency*, N_b is the number of bytes sent and T_b is the time per byte. In terms of *bandwidth* B:

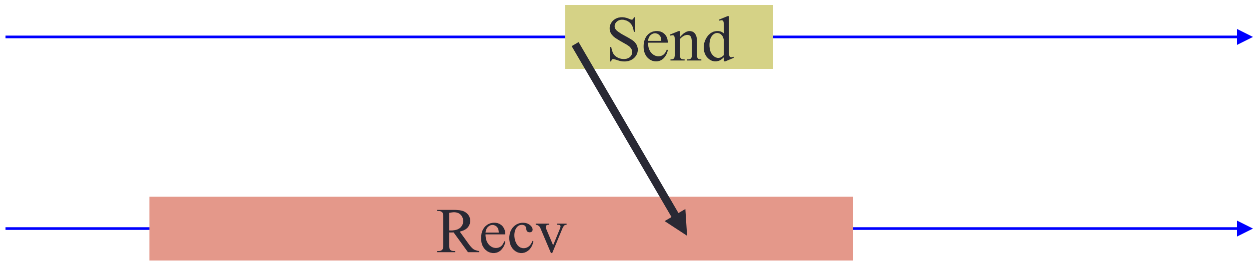
$$T_p = T_l + N_b / B$$

- Faster to send one large message vs many small ones
  - e.g. one allreduce of two doubles vs two allreduces of one double
  - derived data-types can be used to send messages with a mix of types

Communication patterns

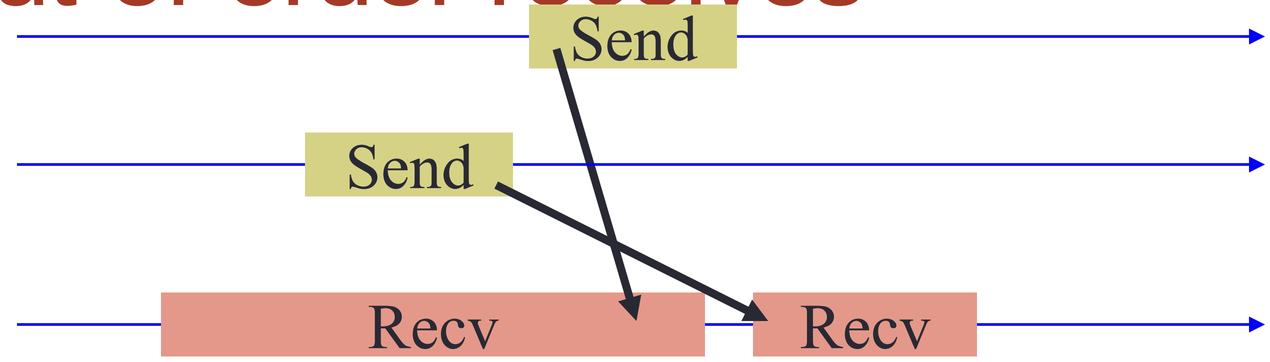
- Can be helpful, especially when using trace analysis tools, to think about communication patterns
  - Note: nothing to do with OO design!
- We can identify a number of patterns which can be the cause of poor performance.
- Can be identified by eye, or potentially discovered automatically
  - e.g. the SCALASCA tool highlights common issues

Late Sender

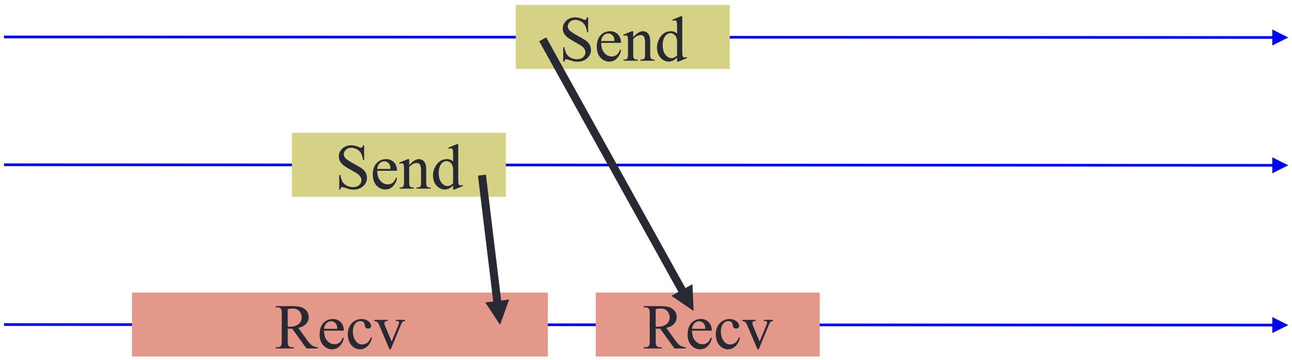


- If blocking receive is posted before matching send, then the receiving task must wait until the data is sent.

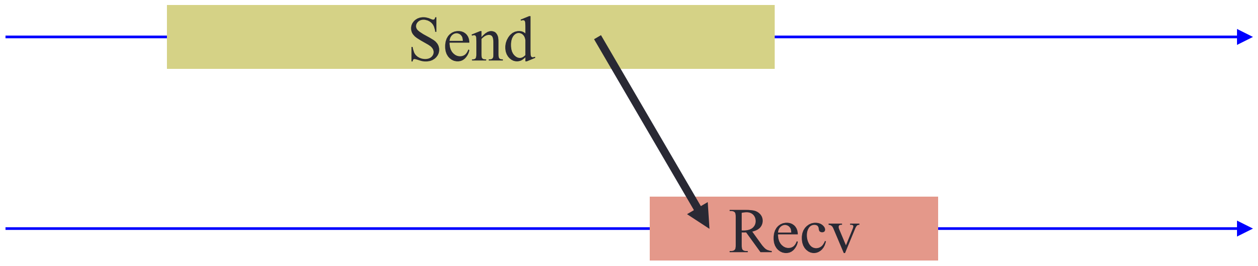
Out-of-order receives



- Late senders may be the result of having blocking receives in the wrong order.



Late Receiver

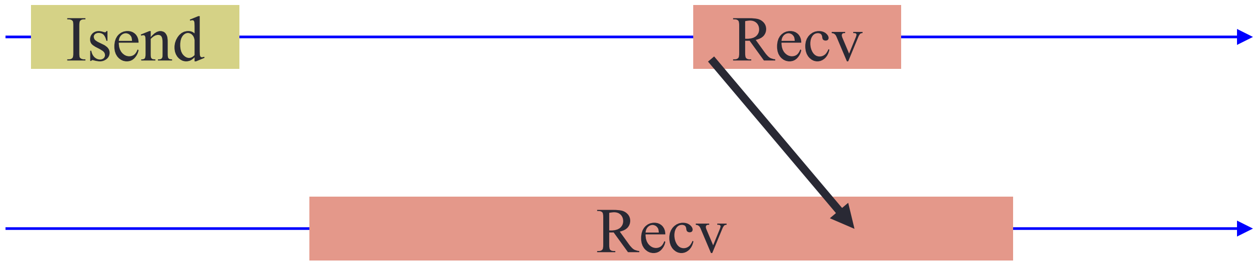


- If send is synchronous, data cannot be sent until receive is posted
  - either explicitly programmed, or chosen by the implementation because message is large
  - sending task is delayed

MPI Progression

- You probably think of MPI as running continuously
  - e.g. asynchronous / non-blocking comms happen “in the background”
  - communications and calculation overlap in time
- This is not generally true
  - MPI library is single-threaded by default, i.e. communications can only be processed when your program calls an MPI function
  - MPI treats calls as manual interrupts and will try to “progress” communications by matching outstanding sends and receives before actually doing what you have asked it to!
- If you issue a non-blocking send
  - it may be sent immediately if there is an existing receive
  - if not, it cannot be sent until the next explicit MPI call (which may be unrelated to the outstanding communication itself)

Late Progress

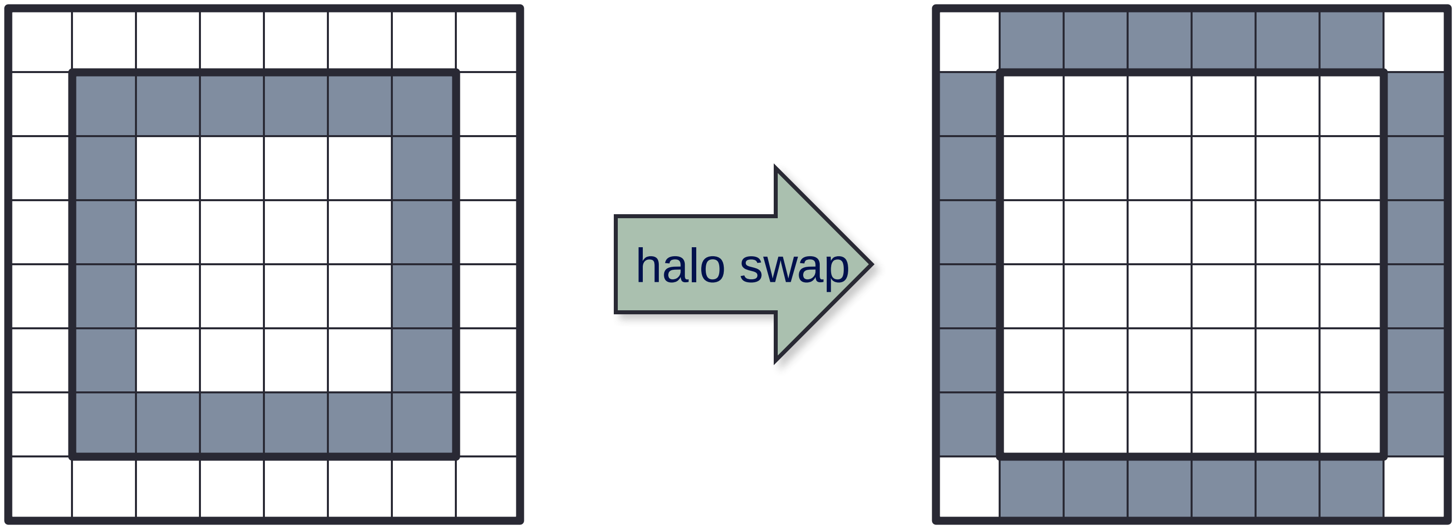


- Non-blocking send returns, but implementation has not yet sent the data.
  - A copy has been made in an internal buffer
- Send is delayed until the MPI library is re-entered by the sender.
  - receiving task waits until this occurs

Non-blocking comms

- Both late senders and late receivers may be avoidable by more careful ordering of computation and communication
- However, these patterns can also occur because of “random noise” effects in the system (e.g. network congestion, OS interrupts)
  - not all tasks take the same time to do the same computation
  - not all messages of the same length take the same time to arrive
- Can be beneficial to avoid delays by using all non-blocking comms entirely (Isend, Irecv, WaitAll)
  - post all the Irecv’s as early as possible

Normal halo swapping




```
swap data into 4 halos: i=0, i=M+1, j=0, j=M+1
loop i=1:M; j=1:N;
   new(i,j) = 0.25*(    old(i-1,j) + old(i+1,j)
                      + old(i,j-1) + old(i,j+1)
                     - edge(i,j)                   )
```

Point-to-point

- Do not impose unnecessary ordering of messages

```
loop over sources:
  receive value from
  particular source;
end loop
```

```
loop over sources:
  receive value from
      any source;
end loop
```

  - loop now just counts the correct number of messages

- Alternative
  - first issue a separate non-blocking receive for each source
  - then issue a single Waitall

Halo swapping

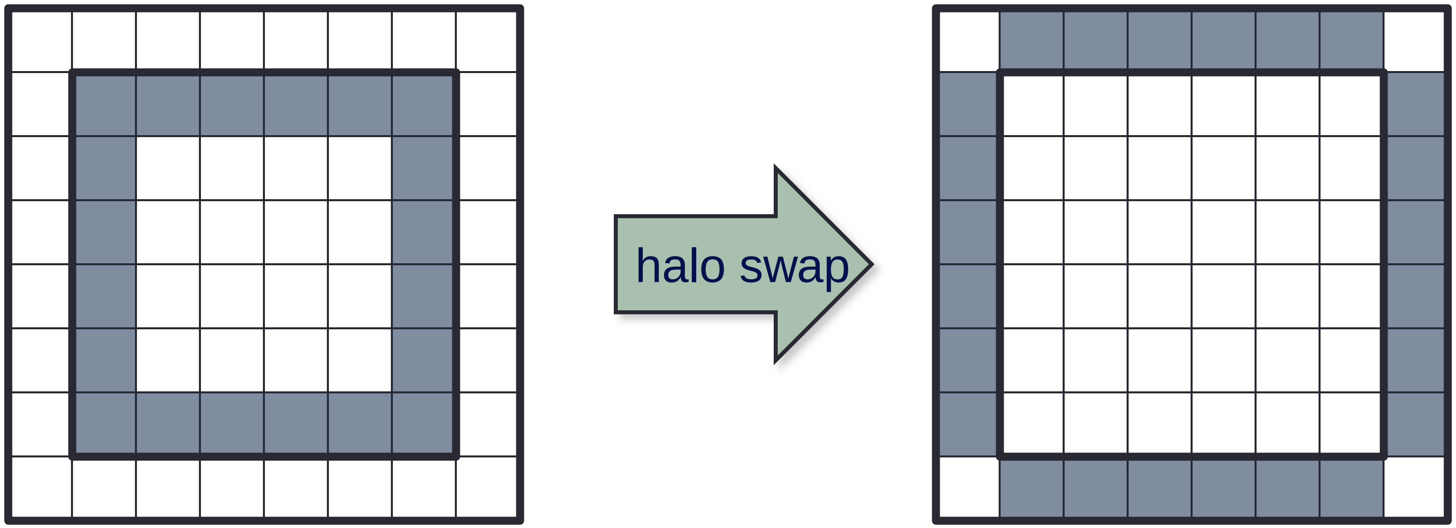
- Do not impose unnecessary ordering of messages

```
loop over directions:
   send up; recv down;
   send down; recv up;
end loop
```

```
loop over directions:
  isend up; irecv down;
  isend down; irecv up;
end loop
wait on all requests;
```

- Extensions
  - can now overlap communications with core calculation
  - only need to wait for receives before non-core calculation
  - wait for sends to complete before starting next core calculation

Overlapping




```
start non-blocking sends/recvs
  loop i=2:M-1; j=2:N-1;
    new(i,j) = 0.25*(   old(i-1,j) + old(i+1,j)
                      + old(i,j-1) + old(i,j+1)
                     - edge(i,j)                )
wait for completion of non-blocking sends/recvs
complete calculation at the four edges
```

epcc

Persistent communications

- Standard method: run this code every iteration

```
MPI_Irecv(..., procup, ..., &reqs[0]);
MPI_Irecv(..., procdn, ..., &reqs[1]);
MPI_Isend(..., procdn, ..., &reqs[2]);
MPI_Isend(..., procup, ..., &reqs[3]);
MPI_Waitall(4, reqs, statuses);
```

- Persistent comms: setup *once*

```
MPI_Recv_init(..., procup, ..., &reqs[0]);
MPI_Recv_init(..., procdn, ..., &reqs[1]);
MPI_Send_init(..., procdn, .... &reqs[2]);
MPI_Send_init(..., procup, ..., &reqs[3]);
```

  - Every iteration:

```
MPI_Startall(4, reqs);
MPI_Waitall (4, reqs, statuses);
```

  - Message ordering *not guaranteed to be preserved*
    - may need to use tags to correctly match messages

Neigbourhood Collectives

- Standard collectives are applied to whole communicator
  - e.g. MPI_Allgather collects data from all *P* processes
- Neighbourhood collectives apply to neighbouring processes
  - e.g. MPI_Neighbor_allgather only collects data from your neighbours
  - requires communicator to be constructed with a topology
- Regular grid
  - Cartesian topology via MPI_Cart_create
  - in 3D grid, gather from six nearest neighbours up, down, left, right, ...
- General communications pattern
  - requires a graph topology
  - each process connected to an arbitrary number of neighbours

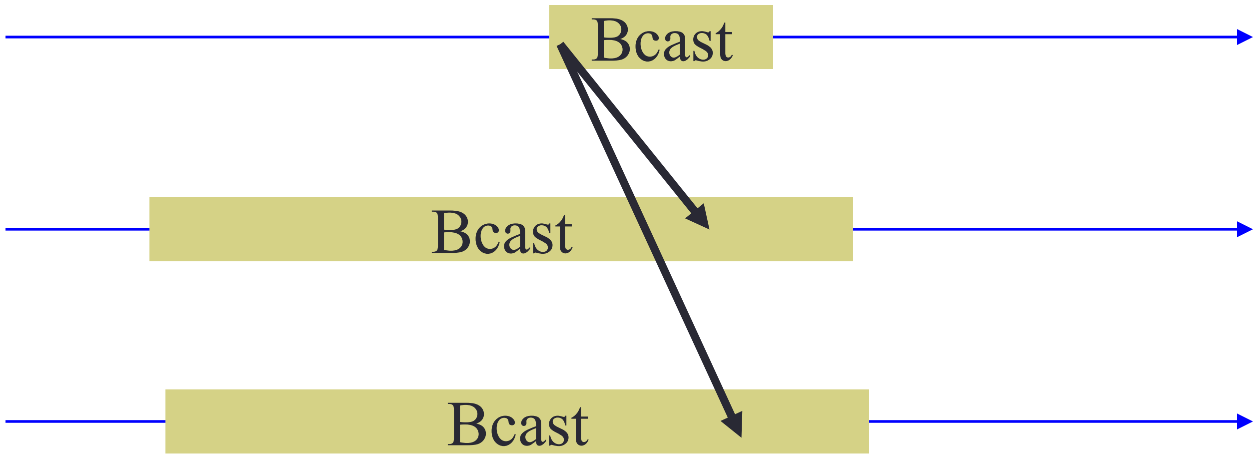
Use for halo swapping

- MPI_Neighbor_alltoall implements halo swapping
  - send and receive data with all your neighbours
- Simple 3D cartesian grid illustrated in halobench exercise
  - for multidimensional arrays need to play tricks with datatypes to send and receive correct data (see later talk)
- MPI library can implement in any way it chooses
  - hopefully efficiently!
  - code is much more elegant and compact than point-to-point

Collective communications

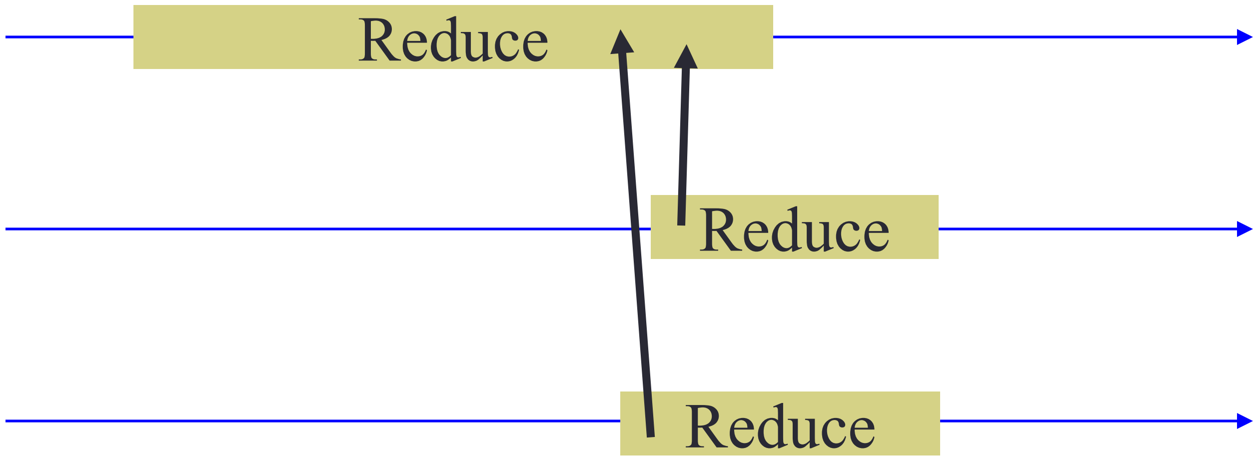
- Can identify similar synchronisation patterns for collective comms as for point-to-point...

Late Broadcaster



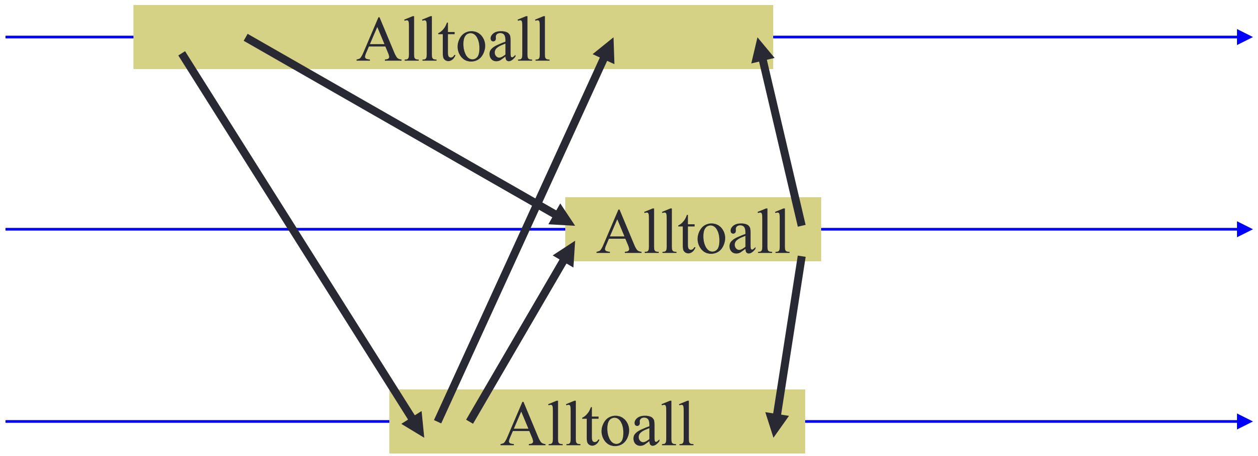
- If broadcast root is late, all other tasks have to wait
- Also applies to Scatter, Scatterv

Early Reduce



- If root task of Reduce is early, it has to wait for all other tasks to enter reduce
- Also applies to Gather, GatherV

Wait at NxN



- Other collectives require all tasks to arrive before any can leave.
  - all tasks wait for last one
- Applies to Allreduce, Reduce_Scatter, Allgather, Allgatherv, Alltoall, Alltoallv

Collectives

- Collective comms are (hopefully) well optimised for the architecture
  - Rarely useful to implement them your self using point-to-point
- However, they are expensive and force synchronisation of tasks
  - helpful to reduce their use as far as possible
  - e.g. in many iterative methods, a reduce operation is often needed to check for convergence
  - may be beneficial to reduce the frequency of doing this, compared to the sequential algorithm
- Non-blocking collectives added in MPI-3
  - may not be that useful in practice …

General advice

- Try to avoid imposing any non-essential message ordering
  - when messages are actually sent can change on every run
- Try to allow MPI to deal with messages as they happen
  - issue all sends and receives as non-blocking
    - issue receives as early as possible
    - complete with a single Waitall()
  - or set up as persistent comms
    - be careful about message ordering
  - or use neigbourhood collectives
- Avoid unnecessary collective calls e.g. by aggregation
  - do you really need any of those barriers?!?

Summary

Can divide overheads up into four main categories:

- Lack of parallelism
  - Cannot split work up into enough pieces
- Load imbalance
  - Pieces for each processor are not identical amount of work
- Synchronisation
  - Processors waiting for each other
- Communication
  - Inefficient patterns of communication